

Influence of Pr ion to electronic structure of oxygen in PrBa₂Cu₃O₇: X-ray fluorescence spectroscopy

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Introduction

PrBa₂Cu₃O₇ is unique in being a semiconductor and not a superconductor having an isostructure with YBa₂Cu₃O₇(Y123), while all the other RBa₂Cu₃O₇ (R=rare-earth element) are superconductors with almost the same critical temperature 90 K [1]. Fehrenbacher and Rice presented a model for this puzzle of high temperature superconductivity in cuprates[2]. They assumes hole depletion in the CuO₂ planes, because of hole transfer from the Cu-O pd σ -band to a hybridized state of Pr 4f and O 2p π orbital (Fehrenbacher-Rice state). Thereafter, Liechtenstein and Mazin calculated the band structure of the state using a tight binding model and showed the presence of the hole state composed of the hybridization state above the Fermi energy[3].

We made previously a polarization analysis of x-ray absorption spectra of oxygen 1s state in PrBa₂Cu₃O₇ [4]. The polarization dependence of the x-ray absorption spectra(XAS) is attributed to the excitation of four inequivalent oxygen sites: O(1) chain, O (2) and O(3) in-plane, and O(4) apical oxygen. Thus, local hole states of the four oxygen were specified. We can probe the local occupied electronic states of the specified oxygen using x-ray emission spectra by the excitation of specified oxygen. Using this technique, we can distinguish the each electronic state of O(2) and O(3) in CuO₂ plane from the other oxygen states. In this paper we report on the influence of Pr ion to electronic state of oxygen on CuO₂ plane in PrBa₂Cu₃O₇ compound based on the x-ray emission measurements of the untwined PrBa₂Cu₃O₇ and YBa₂Cu₃O₇ single crystals.

Experimental

Samples were prepared using a self-flux growth using gold crucibles and annealed in oxygen atmosphere. The specimen was then detwinned by a thermal-mechanical method [5].

The measurements of O K α x-ray emission spectra near the O 1s threshold were performed at the Advanced Light Source on beamline 8.0. The fluorescent radiation emitted from the sample was energy analyzed with a high-resolution grating spectrometer and a computer-interfaced multi-channel detector. The resolution of the beamline monochromator was set to 0.5 eV for 530 eV photon energy. The O K α x-ray emission spectra were recorded using a 1500 lines/mm grating ($R = 10$ m) in the first order of diffraction with the spectrometer resolution set to 0.8 eV.

Results and Discussions

The emission spectra of chain oxygen sites in PrBa₂Cu₃O₇ and YBa₂Cu₃O₇ were same each other and those of apical oxygen sites in these compounds were same also each other. However, the emission spectra of oxygen in CuO₂ plane sites in PrBa₂Cu₃O₇ were different from those of YBa₂Cu₃O₇.

Figure shows the emission spectra of O(2) in plane site of PrBa₂Cu₃O₇ and YBa₂Cu₃O₇.

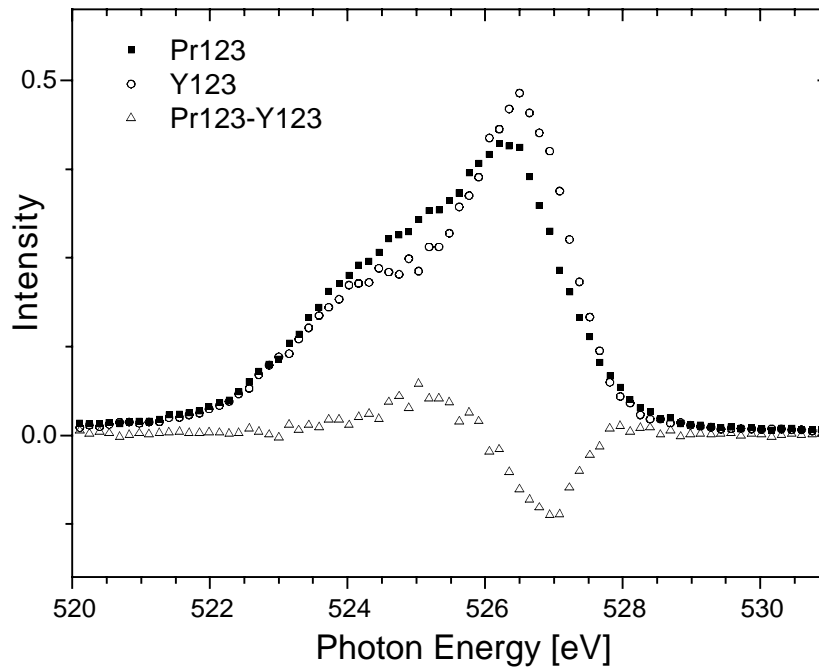


Figure. Emission spectra from oxygen O(2) on CuO₂ plane in PrBa₂Cu₃O₇ and YBa₂Cu₃O₇, and difference between two spectra.

The difference of intensity between two spectra is also plotted in the Figure. Two spectra have peak at about 527eV, which corresponds to non-bonding state of oxygen 2p π . The peak of non-bonding 2p π state in PrBa₂Cu₃O₇ is reduced and broader than that of YBa₂Cu₃O₇. The situation was predicted by the band theoretical calculation by Liechtenstein and Mazin and the difference of the two spectra was consistently compared with their theoretical calculation. This is the evidence of hybridization between the Pr 4f and O p π orbital, which causes suppression of superconductivity in PrBa₂Cu₃O₇.

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